NISTmAb Mass Spectral Reference Libraries: Freely Available



LC-ESI-MS/MS library for detailed mAb characterization

- 3.360 peptides
- 12,608 spectra
- Extensive degradation, glycation, oxidation, and cysteine variation
- Over 20 types of analytical artifacts
- Based on 1D/2D LC-MS studies
- Multiple HCD collisional energies

LC-ESI-MS/MS library for glycoanalysis

- 1,703 spectra
- 247 multiply charged glycopeptides
- 81 different N-glycans (NSO and CHO)
- 20-fraction 2D-LC studies



References

- J. Proteome Res. 2016, 15, 5, 1472-1486
- mAbs, 2018, 10:3, 354-369
- NIST RM 8671: https://www.nist.gov/srm







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How to use libraries

- Formats: (1) ASCII text format (MSP) and
 (2) MS Search binary format
- Library searching with major proteomics workflows, including *Mascot* (Matrix Science) and *Proteome Discoverer* (Thermo Fisher Scientific)
- Individual spectrum search with the full-featured user-interface program: NIST MS Search
- Batch peptide identification with the NIST MS PepSearch software

Library Downloads

Peptide.nist.gov

Web <u>chemdata.nist.gov</u>



Email massspec@nist.gov

